

Power-law Temperature Dependent Hall Angle in the Normal State and its Correlation with Superconductivity in iron-pnictides

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We report Hall measurement of the normal state in K- and Co-doped BaFe₂As₂, as well NaFe_{1-x}Co_xAs. We found that a power-law temperature dependence of Hall angle, $\cot\theta_H \propto T^\beta$, prevails in normal state with temperature range well above the structural, spin-density-wave and superconducting transitions for the all samples with various doping levels. The power β is nearly 4 for the parent compounds and the heavily underdoped samples, while around 3 for the superconducting samples. The β suddenly changes from 4 to 3 at a doping level that is close to the emergence of superconductivity. It suggests that the β of ~ 3 is clearly tied to the superconductivity. Our data suggest that, similar to cuprates, there exists a connection between the physics in the normal state and superconductivity of iron-pnictides. These findings shed light on the mechanism of high-temperature superconductivity.

PACS numbers: 74.62.-c; 74.25.F-; 74.70.Xa

As a second family of high- T_c superconducting materials, iron-pnictides have been frequently compared to high- T_c cuprates [1–4]. There are many similarities between them, such as: an antiferromagnetism in the parent compounds and the quasi-two-dimensional nature of superconducting CuO₂ and FeAs layers. Superconductivity is realized by suppressing the antiferromagnetic (AFM) ground state in both of these superconductors. In cuprates, one of the central puzzles is the unusual properties of the normal states, for instance, pseudogap, linear-temperature dependent resistivity, T^2 behavior of Hall angles, which can give clues to the underlying microscopic interactions and the mechanism of superconductivity [5, 6]. Comparing the two high- T_c families, we are curious about whether the normal states in iron-pnictides can provide some hints and help to uncover the high- T_c physics. In deed, unusual behavior, such as linear-temperature dependence of magnetic susceptibility above the AFM transition [7, 8], strong temperature-dependent Hall coefficients [9–13], has been observed in iron-pnictides. Although the underlying physics is still under debate, these properties are closely related to the multiband character of iron-pnictides that is a crucial key to the understanding of the superconductivity in these materials.

While de Haas-van Alphen and angle-resolved photoemission spectroscopy (ARPES) can precisely determine the Fermi surface topology and the band structure, the electronic transport measurements are more sensitive to the subtle and complicated interactions in the multiband system. In particular, transport measure-

ments can determinately uncover anomalous behavior in the normal states. Here, we will show that resistivity and Hall measurements hint a connection between the high-temperature normal state and the low-temperature superconducting state. We have investigated a series of single crystals of Ba_{1-x}K_xFe₂As₂ and Ba(Fe_{1-x}Co_x)₂As₂, as well NaFe_{1-x}Co_xAs. The cotangent of Hall angle, $\cot\theta_H$, from resistivity and Hall measurements was observed to vary with a simple but systematic trend. The $\cot\theta_H$ shows a fashion of T^β in the paramagnetic state well above the structural, SDW and superconducting transitions. The magnitude of β is ~ 4 in the heavily underdoped regime near the parent compound, while it drops to ~ 3 when the superconducting ground state emerges. With further doping, β remains ~ 3 in a small doping range and then decreases gradually with the vanishing of superconducting ground state. Together with the similar behavior observed in NaFe_{1-x}Co_xAs, our data show a consistent behavior in the high-temperature behavior in the normal state, which bears a connection with the emergence of superconducting ground state.

Figure 1(a) shows the temperature dependence of resistivity for single crystalline Ba_{1-x}K_xFe₂As₂ and Ba(Fe_{1-x}Co_x)₂As₂ with various doping, with a marked asymmetric changes of transport properties induced by electron and hole doping. Our data are similar to previous reports of resistivity in doped BaFe₂As₂ crystals [14, 15]. It is evident that the high-temperature resistivity exhibits distinct curvatures for electron and hole dopings. In the hole-doped region (Fig. 1(a), top panel), the high-temperature curvature is downwards, while it is upwards in the electron-doped region (Fig. 1(a), bottom panel). It is interesting that the high-temperature resistivity of the parent compound bears a similarity to that of electron-doped compounds, which suggests that

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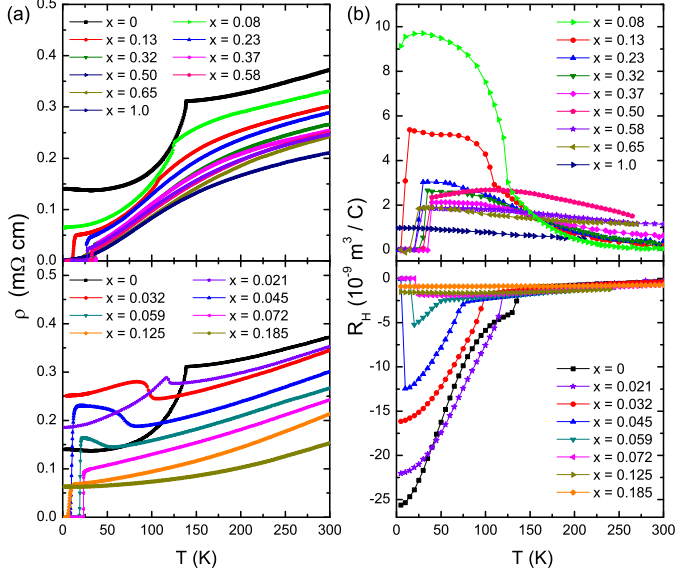


FIG. 1: (Color online) (a): Temperature dependence of resistivity for $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ (top) and $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ (bottom) single crystals, respectively; (b): Temperature dependence of Hall coefficient for $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ (top) and $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ (bottom) single crystals, respectively.

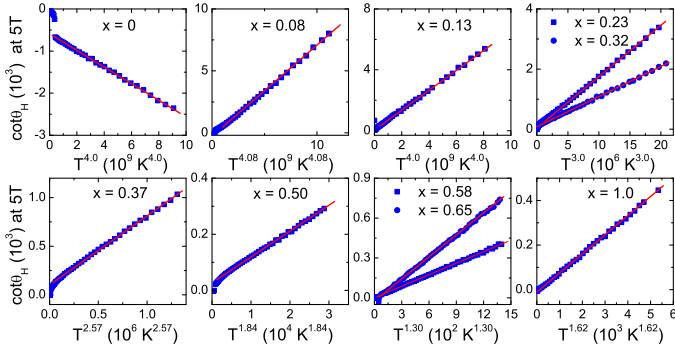


FIG. 2: (Color online) $\cot\theta_H$ vs. T^β for the single crystals of $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ system with different x . The magnitude of β varies from sample to sample. The solid red lines show the T^β dependence of $\cot\theta_H$.

at high temperatures the parent compound can be considered as an electron doped compound. This argument is further reinforced by the results of Hall measurements, which shows that at high temperatures the electron carriers dominate the transport properties in the parent compound (Figure 1(b)).

On the other hand, the transport measurements show complex behavior at low temperatures below the structural and SDW transitions. The resistivity shows different temperature-dependence in the Co and K doping regimes. In fact, it has been found that SDW, electronic nematicity and orbital ordering etc. take place below the structural/SDW transitions [16], which can significantly reconstruct the band structure and give rise to

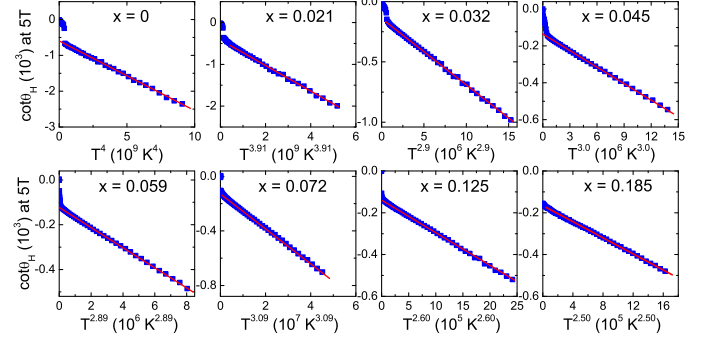


FIG. 3: (Color online) $\cot\theta_H$ vs. T^β for $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ single crystals with various doping. The magnitude of β varies from sample to sample. The solid red lines show the T^β dependence of $\cot\theta_H$.

novel properties in the electronic systems [16]. In this paper, we focus on the data at high temperatures well above the structural and SDW transitions. We stress that, without the driving forces from those ordering tendency, the high-temperature transport data are able to provide information on the fundamental changes in the prime band structure, which can supply valuable information on the physics of iron-pnictides.

Figure 1(b) shows the Hall coefficient R_H for both $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ (top) and $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ (bottom) crystals with various doping. In a typical compensated semimetal, where the densities of electron and hole carriers are roughly equal to each other, a vanishing Hall coefficient R_H is usually expected. However, similar to earlier reports by other groups [9–13], the Hall coefficient R_H shows a strong temperature dependence. In particular, the transport properties seem to be dominated by a single type of carriers in these multiband systems, and a remarkable electron or hole character of transport properties can be induced by a slight electron or hole doping. It is evident that the R_H of $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ is always negative, suggesting the dominance of electron carriers. In $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$, the R_H turns to be positive with slight hole doping ($x \geq 0.08$), showing that the hole carriers govern the transport properties. The significant rise in the magnitude of R_H is associated with the structural/SDW transitions, which is not the focus of the our study here. How to explain the unconventional Hall properties is still under debate. In this paper, we focus on the high temperature region well above the structural, SDW and superconducting transitions.

Despite of its complicated properties, we found that the resistivity and Hall data reveal a intrinsic but simple behavior. Using the resistivity and Hall data displayed in Figs. 1(a) and (b), we can calculate the cotangent of Hall angles, $\cot\theta_H = \rho/\rho_{xy}$, for both $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ and $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ crystals. The Hall angle reveals a power-law temperature dependence, $\cot\theta_H = A + BT^\beta$, in the temperature range well above SDW, structural

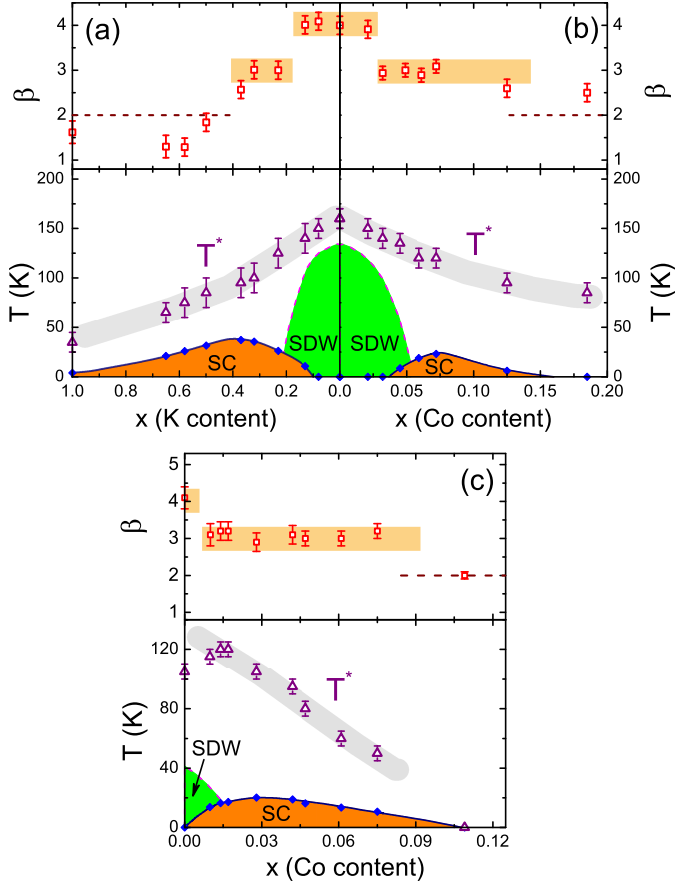


FIG. 4: (Color online) The doping dependence of the power-law exponent β and phase diagrams for **(a)**: $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$, **(b)**: $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ and **(c)**: $\text{NaFe}_{1-x}\text{Co}_x\text{As}$, respectively. The data of $\text{NaFe}_{1-x}\text{Co}_x\text{As}$ are taken from Ref.17. The T^* is the characteristic temperature at which the Hall angles deviate from the high-temperature T^β behavior.

and superconducting transitions. Figures 2 and 3 show the plots of $\cot\theta_H$ vs. T^β for both $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ and $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$, respectively. A T -power law dependence holds for all the crystals at high temperatures. In Figure 2, the $\cot\theta_H$ of the parent compound BaFe_2As_2 decreases with increasing temperature, which is similar to the behavior of electron-doped compounds as shown in Fig. 3. Together with the resistivity data, this behavior suggests that BaFe_2As_2 can be considered as an electron doped compound in the high-temperature normal state. In contrast, the $\cot\theta_H$ in hole-doped samples for $x \geq 0.08$ increases with temperature. Our data indicate that the temperature dependence of the $\cot\theta_H$ can provide information on whether electron or hole carriers predominate the transport properties. Moreover, one may notice that the magnitude of the power β varies from sample to sample. Moreover, such a T^β behavior of Hall angle in the normal state has also been found in Co-doped NaFeAs family, as reported by us in Ref. 17.

For a comparison, the T^β behavior of Hall angle has

been observed in cuprate superconductors, which is considered to be a peculiar properties of the unusual normal state, though the explanation for this behavior is controversial. In most cuprates, T^2 dependence of the $\cot\theta_H$ holds for a wide doping range in the normal state above the pseudogap-opening temperature [6, 18]. In contrast, our data show that the power β varies with doping in iron-pnictides. Together with the phase diagrams, the powers β for the K- and Co-doped BaFe_2As_2 and Co-doped NaFeAs are summarized in Fig. 4. Moreover, we have marked in the phase diagrams the T^* temperatures, below which the Hall angles deviate from the T^β behavior. It is very interesting that the evolutions of T^* with doping show a highly consistent behavior in both of the doped BaFe_2As_2 and NaFeAs families, and further studies are required to show what happens at these crossover temperatures. Systematic measurements by ARPES have shown that the carrier doping induced by K and Co dopants leads to a rigid-band-like change of the valence band structure [19–21]. Therefore, Fig. 4 displays a systematic change of electronic properties due to the variation of electron and hole carriers in BaFe_2As_2 and NaFeAs. It is worth noting that the power-law behavior occurs in high temperature region above the structural, SDW and superconducting transitions, which reveals the fundamental electronic properties of the iron-pnictides without the complexity due to the low-temperature electronic reconstructions.

In Fig. 4, it is remarkable that the variation of the power β behaves in a highly similar fashion in BaFe_2As_2 and NaFeAs families. In the parent compounds of BaFe_2As_2 and NaFeAs, $\beta \sim 4$, and the magnitude of β persists until the emergence of superconductivity. In the doping range where the superconducting ground state prevails, β drops to ~ 3 . Then, $\beta \sim 3$ holds for a wide range of superconducting compounds. With further doping, superconductivity fades away, β decreases to a smaller value. With the emphasis on the consistent variation of β in these materials, we also notice some exceptions. In the parent compound of NaFeAs family, there is no bulk superconductivity, we therefore consider it a non-superconducting compound. In addition, the significant decrease of β in the overdoped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ is likely coincident with the fact that the isotropic gap structure gradually changes to a nodal one with K doping [22, 23], though it is unclear how such a variation can change the magnitude of β .

As already shown in Fig. 1, the electronic transport in electron and hole doped region of BaFe_2As_2 is quite different. Moreover, many properties of NaFeAs family are distinct from those of BaFe_2As_2 compounds. However, the similar doping-dependent variation of β in these materials suggests that there is a connection between the high-temperature transport data and the low-temperature electronic ground states. At high temperatures, the electronic band structure and underlying in-

interactions are relatively simple, without the complexity due to the electronic reconstruction or ordering tendency at low temperatures. With the electron and hole doping, ARPES data have shown that the band structure changes in a rigid-band-like fashion, without significant variation of local correlations [19–21]. Thus, it is reasonable to believe that, at high temperatures, the fundamental change in the electronic system is the shifting of Fermi energy. Generally, one may expect β evolves gradually with carrier doping, since the rigid-band-like change in the band structure is smooth [19–21]. However, the reduction of β from 4 to 3 seems to be a sudden drop, which suggests a particular change of the band structure by either hole or electron doping. It is worth noting that, the electronic properties of electron and hole pockets in iron-pnictides are remarkably different, while our data shows that the Hall angles in the electron- and hole-doped BaFe_2As_2 behave in a similar fashion. This counterintuitive finding suggests that the normal-state electronic structure and its interactions with various degrees of freedom contain important messages about iron-pnictide physics. Unfortunately, there is no high-temperature ARPES data available to unambiguously show the critical change in the band structure [19–21]. We can only infer such a change by the variation of β . The close connection between this reduction of β and the emergence of superconducting ground state suggests that the change of the band structure by doping favors the superconductivity in iron-pnictides. Moreover, Fig. 3 shows that $\beta \sim 3$ is associated with the superconducting ground state, though β decreases continuously with K doping in overdoped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$, which is probably associated with the variation of the gap structure from isotropic to nodal one. In particular in Co-doped BaFe_2As_2 and NaFeAs , $\beta \sim 3$ prevails in the whole superconducting regimes. All these properties point out the high-temperature normal state possesses substantial clues on the superconductivity in iron-pnictides, though it is unclear how the change of the band structure boosts superconductivity in cooperation with spin or orbital degrees of freedom.

Even though the Hall measurements of BaFe_2As_2 and NaFeAs families show unconventional properties that has not been unambiguously explained, the power-law temperature dependence of Hall angles reveal that $\beta \sim 3$ is crucial for superconductivity, which could give a clue on the connection between superconductivity and the complex interactions in iron-pnictides. The electron doped and hole doped iron-pnictide superconductors exhibit distinct Fermi surface topology [19–21], thus one would expect the different transport properties. Surprisingly, the power-law temperature dependence of Hall angles $\beta \sim 3$ in the normal state above a characteristic temperature (T^*) is universal for the superconducting samples. The intrinsic mechanism of this unexpected power-law behavior in the normal state is still unknown, and further works need to do to unveil its origin. Moreover,

superconductivity has been found in Ru and P doped BaFe_2As_2 , in which Ru and P change local interactions in the electronic system. It would be interesting to investigate whether $\beta \sim 3$ is a universal behavior and holds for these materials. These studies, together with our results, will shed light on the roles of charge itinerancy and local interactions in iron-pnictides.

In summary, the Hall angle of $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$, $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ shows a power-law behavior, $\cot\theta_H \propto T^\beta$, at high temperatures well above the structural, SDW and superconducting transitions. $\beta \sim 4$ was observed for the parent compound and the heavily underdoped samples on both the electron and hole doped sides. With increasing doping, as the superconductivity occurs, the β suddenly decreases to ~ 3 . The close connection between the change of β magnitude and the emergence of superconductivity suggest that some important electronic property at high temperatures is crucial for the understanding of the superconductivity in iron-pnictides.

Acknowledgements:

This work is supported by the National Natural Science Foundation of China (Grants No. 11190021, 11174266, 51021091), the "Strategic Priority Research Program (B)" of the Chinese Academy of Sciences (Grant No. XDB04040100), the National Basic Research Program of China (973 Program, Grants No. 2012CB922002 and No. 2011CBA00101), and the Chinese Academy of Sciences.

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